

Tridecane  
629-50-5 | DTXSID6027266

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.33e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.28e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Octane, 1-iodo-</div> <div>Measured: 5.58e-02</div> <div>Predicted: 1.82e-01</div>	<div>Image not found</div> <div>Decanoic acid</div> <div>Measured: 2.08e-01</div> <div>Predicted: 9.27e-04</div>	<div>Image not found</div> <div>Triethylenetetramine</div> <div>Measured: 1.35e-01</div> <div>Predicted: 2.46e-04</div>
<div>Image not found</div> <div>Tridecane</div> <div>Measured: 1.16e-02</div> <div>Predicted: 6.33e-02</div>	<div>Image not found</div> <div>Dodecanenitrile</div> <div>Measured: 6.38e-02</div> <div>Predicted: 5.43e-03</div>	